

On the quantum ground state of some noncentral potentials in two-dimensions

R S Kaushal *

Department of Physics and Astrophysics, University of Delhi, Delhi-110 007, India

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Abstract : Using a simple wellknown prescription, we investigate the possibility of obtaining a normalizable ground state solution to the Schrödinger wave equation for a generalized, noncentral cubic potential in two-dimensions. It is found that such a solution does not exist for the cubic potential in general and for the Henon-Heiles system in particular. Further a large number of noncentral, exponential (Toda-type) potentials, which admit the solution to the wave equation, are suggested.

Keywords : Wave equation, noncentral anharmonic and exponential potentials, normalizable eigensolution, integrability.

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With a view to exploring new features and phenomena (like Berry's phase, quantum chaos etc.) and also a somewhat deeper connection between classical and quantum mechanics, there have been several attempts recently to study the quantum aspect of a system already studied at the classical level. Such studies have been carried out in connection with both [1] classically integrable [2] and nonintegrable [3] systems. The most familiar and well-studied example of a classically nonintegrable system in two-dimensions is that of Henon-Heiles system [4],

$$V(x, y) = (1/2)(x^2 + y^2) + (x^2 y - (1/3)y^3). \quad (1)$$

Interestingly, the noncentral potential (1) represents the truncated form of the Toda potential [5, 6],

$$V(x, y) = \frac{1}{24} \left[\exp(2(y + \sqrt{3}x)) + \exp(2(y - \sqrt{3}x)) + \exp(-4y) \right] - \frac{1}{8}, \quad (2)$$

which is an integrable system in the classical sense. In fact, the classical integrability of a system need not necessarily imply [7] its quantum integrability mainly because of the non-triviality of the relation between the classical Poisson bracket and the corresponding commutator. While this problem of quantum integrability of a given classically integrable system is well pursued, no attempt has been made, to the best of our knowledge, to study the problem of solvability of the Schrodinger equation for such systems.

* UGC Research Scientist

It is rather difficult to visualize the problem of solvability of the Schrödinger equation for central potentials, since for such potentials there always exists an additional symmetry and hence other constants of motion. But for noncentral potentials this is not the case. Even at the classical level it is not always possible to find [5, 6] the second constant of motion for such systems and as such the integrable systems are in scarcity compared to nonintegrable systems. On the other hand, inspite of the fact that the Schrödinger equation remains linear even for all noncentral potentials (unlike the corresponding classical equations of motion), a simple analysis has shown [8] that it does not admit the solution for all such systems.

Earlier, using a simple method [9], we have studied [8] the solvability of the Schrödinger equation for a variety of central and noncentral potentials. While harmonic and quartic-type anharmonic potentials in two-dimensions are investigated in detail, the cubic-type anharmonicity somehow could not be explored to that extent. Particularly, the noncentral potentials of the type

$$V(x,y) = \sum_{i,j=0}^N b_{ij} x^i y^j \quad (i+j \leq N, \text{ (where } i \text{ and } j \text{ are not zero simultaneously)}),$$

for $N=2$ and 4 , are found not to provide a normalizable solution to the wave equation with nonzero eigenvalue unless an inverse harmonic term $(b_1/x^2 + b_2/y^2)$ and/or cross terms of the type $(b_3 x/y + b_4 y/x)$ are added to it. In this way several solvable cases were found which possess a normalizable ground state.

On the other hand, it is well known that the potential (1) as such does not offer specially bounded classical particle orbits [10] and also true quantum bound states [11]. Now question arises whether the cubic potential (1) after the generalization mentioned above (cf. eq. (9) below) can offer a quantum bound state; or like quadratic and quartic potentials, will it now become possible for the potential (9) to possess a normalizable bound state. Furthermore, since the cubic anharmonicity, (particularly of the type (1)), shows some abnormal features at the classical level in terms of integrability, one can again ask whether such features also manifest at the quantum level. With a hope to find answers to these questions, in the present work, we analyse the case of noncentral, cubic potentials in two-dimensions. Besides we also explore the ground states of some noncentral, exponential (Toda-type) potentials. In particular, the solvability of the Schrödinger equation for a noncentral cubic potential of very general nature will be investigated here and the ground state solutions will be obtained for a class of noncentral exponential potentials. As the details of the method have appeared elsewhere [8] we restrict here only to the essential steps.

We consider the solution to the Schrödinger wave equation,

$$\phi_{xx} + \phi_{yy} + [\lambda - v(x,y)] \phi(x,y) = 0, \quad (3)$$

where $\lambda = 2\mu E/\hbar^2$, $v(x,y) = 2\mu V(x,y)/\hbar^2$, with a generalized cubic potential

$$v(x,y) = a_{20}x^2 + a_{02}y^2 + a_{11}xy + a_{30}x^3 + a_{03}y^3 + a_{12}xy^2 + a_{21}x^2y. \quad (4)$$

For the eigenfunction, $\phi(x,y)$, we make an ansatz [8]:

$$\phi(x,y) = \exp(g(x,y)), \quad (5)$$

with $g(x,y) = \beta_{20}x^2 + \beta_{02}y^2 + \beta_{11}xy + \beta_{12}xy^2 + \beta_{21}x^2y + \beta_{30}x^3 + \beta_{03}y^3$,

which implies

$$\phi_{xx} + \phi_{yy} = (g_x^2 + g_y^2 + g_{xx} + g_{yy}) \phi(x,y). \quad (6)$$

A comparison of (6) with (3) yields the following set of equations:

$$\lambda = -(2\beta_{20} + 2\beta_{02}), \quad (7a)$$

$$4\beta_{20}^2 + \beta_{11}^2 = a_{20}; \beta_{11}^2 + 4\beta_{02}^2 = a_{02}; 4\beta_{20}\beta_{11} + 4\beta_{02}\beta_{11} = a_{11} \quad (7b, c, d)$$

$$8\beta_{20}\beta_{21} + 6\beta_{11}\beta_{30} + 4\beta_{02}\beta_{21} + 4\beta_{11}\beta_{12} = a_{21}, \quad (7e)$$

$$4\beta_{20}\beta_{12} + 4\beta_{11}\beta_{21} + 8\beta_{02}\beta_{12} + 6\beta_{11}\beta_{03} = a_{12}, \quad (7f)$$

$$12\beta_{20}\beta_{30} + 2\beta_{11}\beta_{21} = a_{30}; 2\beta_{11}\beta_{12} + 12\beta_{02}\beta_{03} = a_{03}, \quad (7g, h)$$

$$12\beta_{21}\beta_{30} + 4\beta_{21}\beta_{12} = 0; 4\beta_{21}\beta_{12} + 12\beta_{12}\beta_{03} = 0, \quad (7i, j)$$

$$4\beta_{21}^2 + 6\beta_{12}\beta_{30} + 4\beta_{12}^2 + 6\beta_{21}\beta_{03} = 0, \quad (7k)$$

$$9\beta_{30}^2 + \beta_{21}^2 = 0; 9\beta_{03}^2 + \beta_{12}^2 = 0. \quad (7l, m)$$

Now, following the same steps as for the quartic case [8], we look for a simultaneous solution to eqs. (7b) – (7m) to determine β_{ij} 's in terms of a'_{ij} 's. In addition to several other relations, the ones of present interest are those obtained immediately from eqs. (7i, j, l, m) as

$$\beta_{12} = -3\beta_{30}; \beta_{21} = -3\beta_{03}; \beta_{21} = \pm i\beta_{30}; \beta_{12} = \pm i\beta_{03},$$

which in turn lead to $\beta_{03} = \pm i3\beta_{30}; \beta_{21} = \mp i3\beta_{03}$. When these results are substituted in the eigenfunction (5), the normalization integral,

$$\int \int |\phi(x,y)|^2 dx dy = 1, \quad (8)$$

turns into an improper integral. In other words, for the potential (4), the wave eq. (3) does not provide a normalizable solution. However, for the Henon-Heiles system (1) we have $a_{02} = a_{20} = 1/2$, $a_{12} = a_{30} = a_{11} = 0$. As a result, eq. (7d) immediately implies $\beta_{02} = -\beta_{20}$, in addition to the above mentioned relations for β 's. Thus, the eigenvalue λ from eq. (7a) also turns out to be zero.

In the presence of inverse harmonic and crossed terms, the potential (4) can be written as

$$\begin{aligned} v(x,y) = & a_{20}x^2 + a_{02}y^2 + a_{11}xy + a_{30}x^3 + a_{03}y^3 + a_{12}xy^2 + a_{21}x^2y \\ & + \frac{a_1}{x^2} + \frac{a_2}{y^2} + a_3\frac{x}{y} + a_4\frac{y}{x} + a_5\frac{x^2}{y} + a_6\frac{y^2}{x} \end{aligned} \quad (9)$$

and the function $g(x,y)$ in ansatz (5) now takes the form,

$$\begin{aligned} g(x,y) = & \beta_{20}x^2 + \beta_{02}y^2 + \beta_{11}xy + \beta_{21}x^2y + \beta_{12}xy^2 + \beta_{30}x^3 + \beta_{03}y^3 + \beta_1 \ln x \\ & + \beta_2 \ln y. \end{aligned} \quad (10)$$

Using (10) in (6) and comparing the resultant equation with (3) for the potential (9), one obtains a set of 19 equations connecting β 's and a 's and one equation for λ . These equations when solved for β 's, also include relations $\beta_{12} = \pm 3i\beta_{03} = -3\beta_{30}$, $\beta_{21} = \pm 3i\beta_{30} = -3\beta_{03}$, alongwith other relations discussed earlier [8]. These results, however, remain unaltered even for the potential (1). Following the same arguments as before, we find again that eq. (3) does not admit a normalizable solution for the potential (9). This situation is somewhat different from that of harmonic and quartic type anharmonic potentials. In fact, in these latter cases the inclusion of inverse harmonic and crossed terms not only led [8] to normalizable solutions but also to nonzero ground state energies.

Next, we proceed to find the ground state for a class of Toda-type potentials. In this case, we slightly depart from our standard method followed earlier [8] in the sense that instead of starting with a known form of the potential in advance, we shall determine the potential itself that can provide a solution to the wave eq. (3). For the function $g(x,y)$ in ansatz (5), we now set

$$g(x,y) = \beta_1 x + \beta_2 y + \beta_3 \exp(\alpha_1 x) + \beta_4 \exp(\alpha_2 y) + \beta_5 \exp(\alpha_3 x + \alpha_4 y), \quad (11)$$

and rewrite eq. (6) in the form

$$\begin{aligned} \phi_{xx} + \phi_{yy} = & [(\beta_1^2 + \beta_2^2) + \beta_3^2 \alpha_1^2 \exp(2\alpha_1 x) + \beta_4^2 \alpha_2^2 \exp(2\alpha_2 y) + \\ & + \beta_5 \alpha_1 (2\beta_1 + \alpha_1) \exp(\alpha_1 x) + \beta_4 \alpha_2 (2\beta_2 + \alpha_2) \exp(\alpha_2 y) + \\ & + \beta_5^2 (\alpha_3^2 + \alpha_4^2) \exp(2(\alpha_3 x + \alpha_4 y)) + \\ & + \beta_5 (2\beta_1 \alpha_3 + 2\beta_2 \alpha_4 + \alpha_3^2 + \alpha_4^2) \exp(\alpha_3 x + \alpha_4 y) + \\ & + 2\beta_3 \beta_5 \alpha_1 \alpha_3 \exp\{(\alpha_1 + \alpha_3)x + \alpha_4 y\} + 2\beta_4 \beta_5 \alpha_2 \alpha_4 \exp\{\alpha_3 x + (\alpha_2 + \alpha_4)y\}]. \\ & \cdot \phi(x,y). \end{aligned} \quad (12)$$

A comparison of eq. (12) with eq. (3) yields an expression

$$\lambda = -(\beta_1^2 + \beta_2^2), \quad (13)$$

for the eigenvalues, and an expression for the potential :

$$\begin{aligned}
 v(x,y) = & \beta_3^2 \alpha_1^2 \exp(2\alpha_1 x) + \beta_4^2 \alpha_2^2 \exp(2\alpha_2 y) + \beta_3 \alpha_1 (2\beta_1 + \alpha_1) \exp(\alpha_1 x) \\
 & + \beta_4 \alpha_2 (2\beta_2 + \alpha_2) \exp(\alpha_2 y) + \beta_5^2 (\alpha_3^2 + \alpha_4^2) \exp(2(\alpha_3 x + \alpha_4 y)) + \\
 & + \beta_5 (2\beta_1 \alpha_3 + 2\beta_2 \alpha_4 + \alpha_3^2 + \alpha_4^2) \exp(\alpha_3 x + \alpha_4 y) + \\
 & + 2\beta_3 \beta_5 \alpha_1 \alpha_3 \exp[(\alpha_1 + \alpha_3)x + \alpha_4 y] + \\
 & 2\beta_4 \beta_5 \alpha_2 \alpha_4 \exp[\alpha_3 x + (\alpha_2 + \alpha_4)y],
 \end{aligned} \tag{14}$$

which admit the solution to eq. (3). Now, we discuss some interesting special cases of potential (14).

Case (1): When $\beta_1 = -\alpha_1/2$, $\beta_2 = -\alpha_2/2$; $\alpha_1 = \alpha_3$, $\alpha_2 = \alpha_4$, the potential (14) reduces to the form

$$\begin{aligned}
 v(x,y) = & \alpha_1^2 [\beta_3 \exp(\alpha_1 x) + \beta_5 \exp(\alpha_1 x + \alpha_2 y)]^2 + \alpha_2^2 [\beta_4 \exp(\alpha_2 y) + \\
 & \beta_5 \exp(\alpha_1 x + \alpha_2 y)]^2,
 \end{aligned} \tag{15}$$

and the corresponding eigenvalue and eigenfunction are given by

$$\begin{aligned}
 \lambda = & -(\alpha_1^2 + \alpha_2^2)/4 \\
 \phi(x,y) = & N. \exp\left[-\frac{1}{2}\alpha_1 x - \frac{1}{2}\alpha_2 y + \beta_3 \exp(\alpha_1 x) + \beta_4 \exp(\alpha_2 y) + \right. \\
 & \left. \beta_5 \exp(\alpha_1 x + \alpha_2 y)\right],
 \end{aligned} \tag{15a}$$

where the normalization constant, N , can be determined from (8).

However, for the choice $\alpha_1 = -\alpha_3$, $\alpha_2 = -\alpha_4$, potential (14) takes the form

$$\begin{aligned}
 v(x,y) = & \alpha_1^2 [\beta_3 \exp(\alpha_1 x) - \beta_5 \exp(-\alpha_1 x - \alpha_2 y)]^2 + \\
 & + \alpha_2^2 [\beta_4 \exp(\alpha_2 y) - \beta_5 \exp(-\alpha_1 x - \alpha_2 y)]^2 + \\
 & 2\beta_5 (\alpha_1^2 + \alpha_2^2) \exp(-\alpha_1 x - \alpha_2 y),
 \end{aligned} \tag{16}$$

while the eigenvalue λ is again given by (15a), $\phi(x,y)$ can be obtained from (11) as before.

Case (2): When $\beta_3 = 0$; $\beta_2 = -\alpha_2/2$, and $\beta_1 = -(\alpha_3^2 + \alpha_4^2 - \alpha_2 \alpha_4)/(2\alpha_1)$, we discuss

here two further choices :

(i) If $\alpha_1 = \alpha_3$, then $\beta_2 = -\alpha_4/2$, and potential (14) becomes

$$v(x,y) = \alpha_2^2 | \beta_4 \exp(\alpha_2 y) + \beta_5 \exp(\alpha_1 x + \alpha_2 y) |^2 + \beta_5^2 \alpha_3^2 \exp(2(\alpha_3 x + \alpha_2 y)). \quad (17)$$

Accordingly, λ and $\phi(x,y)$ are given by

$$\lambda = -\frac{1}{4}(\alpha_3^2 + \alpha_2^2); \phi(x,y) = N \exp \left[-\frac{1}{2} \alpha_1 x - \frac{1}{2} \alpha_2 y + \beta_4 \exp(\alpha_2 y) + \beta_5 \exp(\alpha_3 x + \alpha_2 y) \right],$$

(ii) If $\alpha_2 = -\alpha_4$, then $\beta_1 = -(\alpha_3^2 + 2\alpha_2^2)/(2\alpha_3)$, the potential becomes

$$v(x,y) = \alpha_2^2 | (\beta_3 \exp(\alpha_2 y) - \beta_5 \exp(\alpha_3 x - \alpha_2 y)) |^2 + \beta_5^2 \alpha_3^2 \exp(2(\alpha_3 x - \alpha_2 y)), \quad (18)$$

With $\lambda = -(\alpha_3^2 + \alpha_2^2)(\alpha_3^2 + 4\alpha_2^2)/(4\alpha_3^2) \rightarrow$, and $\phi(x,y)$ can be derived from (11).

Case (3). When $\beta_4 = 0$; $\beta_1 = -\alpha_1/2$; $\beta_2 = -(\alpha_3^2 + \alpha_4^2 - \alpha_1 \alpha_3)/(2\alpha_4)$, we again discuss two choices:

(i) If $\alpha_1 = \alpha_3$, then $\beta_2 = -\alpha_4/2$, and potential (14) becomes

$$v(x,y) = \alpha_1^2 | \beta_3 \exp(\alpha_1 x) + \beta_5 \exp(\alpha_1 x + \alpha_3 y) |^2 + \beta_5^2 \alpha_4^2 \exp(2(\alpha_1 x + \alpha_4 y)), \quad (19)$$

with the eigenvalue, $\lambda = -(\alpha_1^2 + \alpha_4^2)/4$, and the eigenfunction $\phi(x,y)$ is given by (11) as before.

(ii) If $\alpha_1 = -\alpha_3$, then $\beta_2 = -(2\alpha_1^2 + \alpha_4^2)/(2\alpha_4)$, and potential (14) now becomes

$$v(x,y) = \alpha_1^2 | \beta_3 \exp(\alpha_1 x) - \beta_5 \exp(-\alpha_1 x + \alpha_4 y) |^2 + \beta_5^2 \alpha_4^2 \exp(-2\alpha_1 x + 2\alpha_4 y), \quad (20)$$

with $\lambda = -(\alpha_1^2 + \alpha_4^2)(\alpha_4^2 + 4\alpha_1^2)/(4\alpha_4^2)$ and $\phi(x,y)$ can be determined from (11) as before.

Although the basic structure of potentials (15) – (20) is fixed by way of obtaining them as special cases of potential (14), still their generalized character can be noticed in terms of the remaining parameters. Further, for real α_i 's they all seem to possess bound and normalizable ground states. In spite of the fact that Toda potential (2) as such could not be accommodated in the structure (14), three-term Toda-type potentials (cf. cases (2)) which admit the solution to eq. (3), are derived. In fact, for suitable choices of β_i 's and α_i 's in (17) and (18), one can obtain potentials, which are very much similar to potential (2). Similarly, a class of Morse-type potentials in two-dimensions which admit the solution to eq. (3) can be derived from the potential (14) itself.

We have seen that the wave eq. (3) does not have a normalizable solution for the cubic potential (9). On this score, one can question the ansatz (5) itself. In fact, even if one starts with an ansatz of the type,

$$\phi(x, y) = f(x, y) \exp(g(x, y)), \quad (21)$$

where $f(x, y)$ is a polynormal and $g(x, y)$ is again given by (10), it is not difficult to visualize that the exponential function in (21) is still responsible for describing the well-behaving nature of the solution $\phi(x, y)$ at $x, y \rightarrow \infty$, and the β_1 - and β_2 -terms in it at $x, y \rightarrow 0$. This clearly justifies the ansatz (5) for $\phi(x, y)$ at least for the purposes of studying the ground state in the present method. Doubts can also be raised about various terms in ansatz (5) (or in ansatz (10) for that matter). As a matter of fact, in order to retain cubic terms in $v(x, y)$, the presence of β_{30} - and β_{03} -terms in $g(x, y)$ is unavoidable and the presence of these latter terms in $g(x, y)$ gives rise to quartic terms in $v(x, y)$. These quartic terms, in the present case, are however absent as we consider only the cubic anharmonicity. As a result, one arrives at the equations of the type (7 l, m), which in turn lead to nonnormalizability of the eigenfunction.

To summarize, we have explicitly shown that unlike noncentral harmonic and quartic potentials, the cubic potential (1) even after generalizing to the form (9) does not possess a normalizable quantum state within the framework of the ansatz (5) or (21). The normalizable ground states however exist and are constructed explicitly for a class of noncentral, exponential potentials. Some of these results may be useful in solid state physics, quantum chemistry and field theories in two-space dimensions. Further the solvability of the Schrödinger equation should not be taken as granted for all noncentral potentials and to some extent it appears that the abnormal features, which a system exhibits at the classical level are carried over to the quantum level also. Finally, it may be of interest to study the classical integrability by way of constructing the second constant of motion for the solvable cases obtained here and earlier in Ref. (8). Such studies are in progress.

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